

Chlorhexidine diacetate  
56-95-1 | DTXSID7032345

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 145 °C

Global applicability domain: Outside

Local applicability domain index: 7.69e-02

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chlorhexidine</div> <div>Measured: 134</div> <div>Predicted: 145</div>	<div>Image not found</div> <div>Chlorhexidine diacetate</div> <div>Measured: 155</div> <div>Predicted: 145</div>	<div>Image not found</div> <div>Amiloride</div> <div>Measured: 241</div> <div>Predicted: 174</div>
<div>Image not found</div> <div>Phenformin</div> <div>Measured: 177</div> <div>Predicted: 169</div>	<div>Image not found</div> <div>1-(o-Tolyl)biguanide</div> <div>Measured: 144</div> <div>Predicted: 150</div>	